EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1	("20050009934").PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2006/03/28 11:25
L2	77626	adduct$3	US-PGPUB; USPAT; USOCR	OR	ON	2006/03/28 11:05
L3	1	1 and 2	US-PGPUB; USPAT; USOCR	OR	ON	2006/03/28 11:05
L4	1	("20030087969").PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2006/03/28 11:27
L5	1	2001US-0909555.ap,prai.	EPO; JPO; DERWENT	OR	ON	2006/03/28 11:57
L6	2	(("6492559") or ("6051056")).PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2006/03/28 11:50
L7	1	("6717019").PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2006/03/28 11:50
L8	123	LASSILA-K$.in. SLONE-C$.in. SASSANO-S$.in. "SASSANO SLONE"-C$.in.	EPO; JPO; DERWENT	OR	ON	2006/03/28 12:41
L9	1	("4311618").PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2006/03/28 12:41

10/618117

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptau223dxm

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 15:47:40 ON 28 MAR 2006
FILE 'REGISTRY' ENTERED AT 15:47:40 ON 28 MAR 2006
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.20	2.41

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

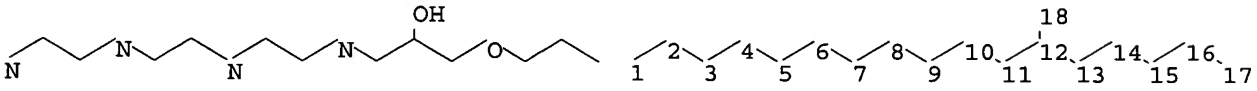
=> screen 1701 AND 1995 AND 2007

L15 SCREEN CREATED

=> screen 1996

L16 SCREEN CREATED

=>
Uploading C:\Program Files\Stnexp\Queries\618117.str



chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 12-18 13-14 14-15 15-16 16-17
exact/norm bonds :
1-2 3-4 4-5 6-7 7-8 9-10 10-11 12-18 13-14 14-15
exact bonds :
2-3 5-6 8-9 11-12 12-13 15-16 16-17

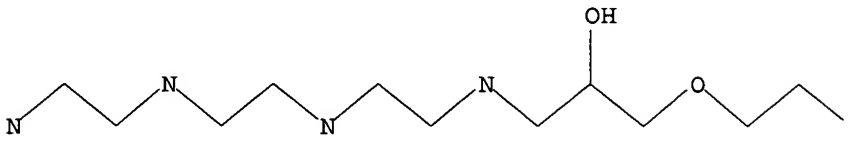
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L17 STRUCTURE UPLOADED

=> que L17 AND L15 NOT L16

L18 QUE L17 AND L15 NOT L16

=> d l18
L18 HAS NO ANSWERS
L15 SCR 1701 AND 1995 AND 2007
L16 SCR 1996
L17 STR



Structure attributes must be viewed using STN Express query preparation.
L18 QUE L17 AND L15 NOT L16

=> s sample sss l18
SAMPLE SEARCH INITIATED 15:48:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 243 TO 877
PROJECTED ANSWERS: 0 TO 0

L19 0 SEA SSS SAM L17 AND L15 NOT L16

=> s l18 sss full
FULL SEARCH INITIATED 15:48:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 649 TO ITERATE

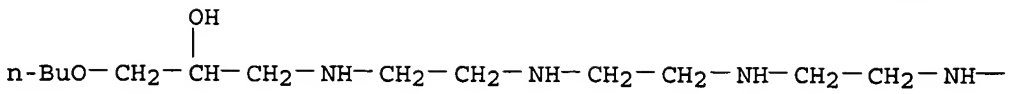
100.0% PROCESSED 649 ITERATIONS 12 ANSWERS
SEARCH TIME: 00.00.01

L20 12 SEA SSS FUL L17 AND L15 NOT L16

=> d 1-12 all

L20 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 490035-28-4 REGISTRY
ED Entered STN: 14 Feb 2003
CN 5,22-Dioxa-9,12,15,18-tetraazahexacosane-7,20-diol (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H46 N4 O4
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); PRP (Properties); USES (Uses)

PAGE 1-A



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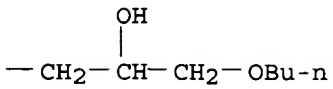

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 10 25 deg C	(1)
Boiling Point (BP)	541.2+/-50.0 deg C	760 Torr	(1)
Density (DEN)	1.010+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	94.17+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	281.1+/-30.1 deg C		(1)
Freely Rotatable Bonds (FRB)	25		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	6		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	14		(1)
Koc (KOC)	1.0	pH 1 25 deg C	(1)
Koc (KOC)	1.0	pH 2 25 deg C	(1)
Koc (KOC)	1.0	pH 3 25 deg C	(1)
Koc (KOC)	1.0	pH 4 25 deg C	(1)
Koc (KOC)	1.0	pH 5 25 deg C	(1)
Koc (KOC)	1.0	pH 6 25 deg C	(1)
Koc (KOC)	1.0	pH 7 25 deg C	(1)
Koc (KOC)	1.0	pH 8 25 deg C	(1)
Koc (KOC)	2.53	pH 9 25 deg C	(1)
Koc (KOC)	20.76	pH 10 25 deg C	(1)
logD (LOGD)	-5.63	pH 1 25 deg C	(1)
logD (LOGD)	-5.46	pH 2 25 deg C	(1)
logD (LOGD)	-4.99	pH 3 25 deg C	(1)
logD (LOGD)	-4.67	pH 4 25 deg C	(1)
logD (LOGD)	-4.39	pH 5 25 deg C	(1)

logD (LOGD)	-3.90	pH 6 25 deg C	(1)
logD (LOGD)	-3.57	pH 7 25 deg C	(1)
logD (LOGD)	-2.36	pH 8 25 deg C	(1)
logD (LOGD)	-0.77	pH 9 25 deg C	(1)
logD (LOGD)	0.14	pH 10 25 deg C	(1)
logP (LOGP)	0.441+/-0.781	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	4.1 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	69 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	8.5 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	4.5 g/L	Unbuffered Water pH 10.99 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.010 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	2.46 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.17 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.021 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.011 mol/L	Unbuffered Water pH 10.99 25 deg C	(1)
Molar Volume (MVOL)	402.4+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	406.60		(1)
pKa (PKA)	13.73+/-0.20	Most Acidic 25 deg C	(1)
pKa (PKA)	9.88+/-0.19	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	107.04 A**2		(1)
Vapor Pressure (VP)	5.73E-14 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:124243 CA
TI Production of alkyl glycidyl ether-capped polyamine antifoaming agents
IN Sassano, Slone Caroline; Lassila, Kevin Rodney
PA Air Products and Chemicals, Inc., USA

SO Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C11D003-00
ICS C11D003-37
CC 46-4 (Surface Active Agents and Detergents)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 1277829	A2	20030122	EP 2002-15652	20020716
EP 1277829	A3	20030502		
EP 1277829	B1	20051019		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2003087969	A1	20030508	US 2001-909555	20010720
US 6656977	B2	20031202		
BR 2002002690	A	20030513	BR 2002-2690	20020715
AT 307182	E	20051115	AT 2002-15652	20020716
CN 1398657	A	20030226	CN 2002-126516	20020719
JP 2003080006	A2	20030318	JP 2002-210403	20020719

PRAI US 2001-909555 20010720
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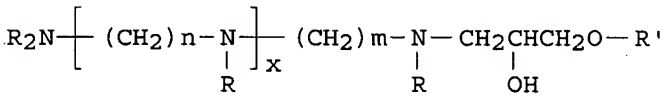


I

AB The foaming of an aqueous composition or an industrial process is controlled by the incorporation of a foam controlling agent having the general formula (I), where n and m are 2 or 3, x is 1-6, R is hydrogen or -CH2-CH(OH)-CH2-O-R', and R' is a C4-C22-alkyl group, the compound I being capable of generating an initial foam height at least 30% less than a 0.1% aqueous solution of dioctyl sodium sulfosuccinate (DOSS) when added at 0.1% to the DOSS solution The alkyl glycidyl ether-capped polyamine antifoaming agents can be used in water-thinned coating compns., inks, agricultural or adhesive compns., or in pulp and paper processing, wastewater treatment, textile dyeing and petroleum gas scrubbing. Thus, 1:1 adduct of diethylenetriamine and Bu glycidyl ether (BGE) was produced by adding one equivalent of BGE to diethylenetriamine at a rate allowing to keep the reaction mixture temperature between 90 and 120°, followed by heating the mixture at 100° for 40 min.

ST nonpolymeric polyamine alkyl glycidyl ether deriv antifoaming agent prodn

IT Ethers, uses
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(glycidyl, C12-C16-alkyl, reaction products with nonpolymeric polyamines; production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT Wetting agents
(nonionic; production of alkyl glycidyl ether-capped polyamines suitable for use as)

IT Amines, uses
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or

engineered material use); PREP (Preparation); USES (Uses)
(polyamines, nonpolymeric, reaction products with alkyl glycidyl ethers; production of alkyl glycidyl ether-capped polyamine antifoaming agents)

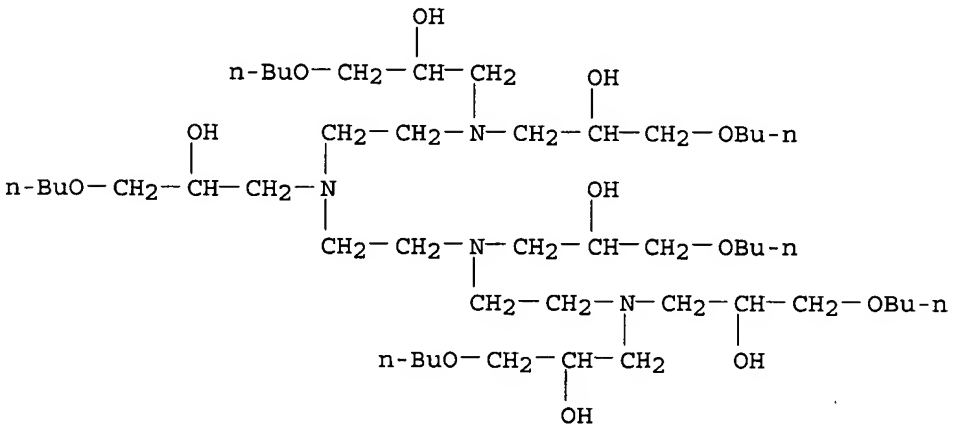
IT Antifoaming agents
Surfactants
(production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 56-18-8DP, reaction products with alkyl glycidyl ethers 112-24-3DP, reaction products with alkyl glycidyl ethers 63888-68-6P 488783-16-0P 488783-17-1P 488783-18-2P 488783-19-3P 488783-20-6P 488783-21-7P 488803-37-8P 490035-26-2P 490035-27-3P 490035-28-4P 490035-29-5P 490035-30-8P 491577-26-5P 491577-27-6P 491577-28-7P 491577-29-8P 491577-30-1P 491577-31-2P 491577-32-3P 491577-33-4P
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 56-18-8, Di(3-aminopropyl)amine 111-40-0, Diethylenetriamine 112-24-3, Ancamine TETA 2426-08-6, Epodil 741 2461-15-6, Epodil 746 160338-56-7, Epodil 748
RL: RCT (Reactant); RACT (Reactant or reagent)
(production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 577-11-7, Dioctyl sodium sulfosuccinate
RL: TEM (Technical or engineered material use); USES (Uses)
(suppression of foam of; production of alkyl glycidyl ether-capped polyamine antifoaming agents)

L20 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 488783-18-2 REGISTRY
ED Entered STN: 12 Feb 2003
CN 5,22-Dioxa-9,12,15,18-tetraazahexacosane-7,20-diol, 9,12,15,18-tetrakis(3-butoxy-2-hydroxypropyl)- (9CI) (CA INDEX NAME)
MF C48 H102 N4 O12
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); PRP (Properties); USES (Uses)



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	22.22	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	66.66	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	131.49	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	393.39	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	947.18	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	11222.53	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	617989.75	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1000000.0	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	1000000.0	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1000000.0	pH 10 25 deg C	(1)
Boiling Point (BP)	899.0+/-65.0 deg C	760 Torr	(1)
Density (DEN)	1.059+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	148.39+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	497.5+/-34.3 deg C		(1)
Freely Rotatable Bonds (FRB)	57		(1)
H acceptors (HAC)	16		(1)
H donors (HD)	6		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	22		(1)
Koc (KOC)	7.54	pH 1 25 deg C	(1)
Koc (KOC)	22.62	pH 2 25 deg C	(1)
Koc (KOC)	44.62	pH 3 25 deg C	(1)
Koc (KOC)	133.48	pH 4 25 deg C	(1)
Koc (KOC)	321.38	pH 5 25 deg C	(1)
Koc (KOC)	3807.86	pH 6 25 deg C	(1)
Koc (KOC)	209686.92	pH 7 25 deg C	(1)
Koc (KOC)	2210920.00	pH 8 25 deg C	(1)
Koc (KOC)	3759676.50	pH 9 25 deg C	(1)
Koc (KOC)	4000701.25	pH 10 25 deg C	(1)
logD (LOGD)	3.88	pH 1 25 deg C	(1)
logD (LOGD)	4.36	pH 2 25 deg C	(1)
logD (LOGD)	4.66	pH 3 25 deg C	(1)
logD (LOGD)	5.13	pH 4 25 deg C	(1)
logD (LOGD)	5.51	pH 5 25 deg C	(1)
logD (LOGD)	6.59	pH 6 25 deg C	(1)
logD (LOGD)	8.33	pH 7 25 deg C	(1)
logD (LOGD)	9.35	pH 8 25 deg C	(1)
logD (LOGD)	9.58	pH 9 25 deg C	(1)
logD (LOGD)	9.61	pH 10 25 deg C	(1)
logP (LOGP)	9.613+/-0.718	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.021 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	630 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	250 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	17 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.29 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.027 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.016 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.015 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.018 g/L	Unbuffered Water pH 8.55	(1)

		25 deg C	
Molar Intrinsic Solubility (ISLB.MOL)	0.000023 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	1.08 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.08 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.08 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.68 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.27 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.018 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00031 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000029 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000017 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000019 mol/L	Unbuffered Water pH 8.55 25 deg C	(1)
Molar Volume (MVOL)	875.3+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	927.34		(1)
pKa (PKA)	13.36+/-0.20	Most Acidic 25 deg C	(1)
pKa (PKA)	7.74+/-0.50	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	189.72 A**2		(1)
Vapor Pressure (VP)	0 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:124243 CA
TI Production of alkyl glycidyl ether-capped polyamine antifoaming agents
IN Sassano, Slone Caroline; Lassila, Kevin Rodney
PA Air Products and Chemicals, Inc., USA
SO Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C11D003-00
ICS C11D003-37
CC 46-4 (Surface Active Agents and Detergents)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1277829	A2	20030122	EP 2002-15652	20020716
	EP 1277829	A3	20030502		
	EP 1277829	B1	20051019		
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	US 6656977	B2	20031202		
	BR 2002002690	A	20030513	BR 2002-2690	20020715
	AT 307182	E	20051115	AT 2002-15652	20020716
	CN 1398657	A	20030226	CN 2002-126516	20020719

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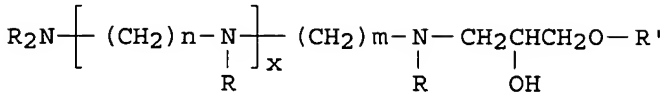


I

AB The foaming of an aqueous composition or an industrial process is controlled by the incorporation of a foam controlling agent having the general formula (I), where n and m are 2 or 3, x is 1-6, R is hydrogen or -CH2-CH(OH)-CH2-O-R', and R' is a C4-C22-alkyl group, the compound I being capable of generating an initial foam height at least 30% less than a 0.1% aqueous solution of dioctyl sodium sulfosuccinate (DOSS) when added at 0.1% to the DOSS solution The alkyl glycidyl ether-capped polyamine antifoaming agents can be used in water-thinned coating compns., inks, agricultural or adhesive compns., or in pulp and paper processing, wastewater treatment, textile dyeing and petroleum gas scrubbing. Thus, 1:1 adduct of diethylenetriamine and Bu glycidyl ether (BGE) was produced by adding one equivalent of BGE to diethylenetriamine at a rate allowing to keep the reaction mixture temperature between 90 and 120°, followed by heating the mixture at 100° for 40 min.

ST nonpolymeric polyamine alkyl glycidyl ether deriv antifoaming agent prodn

IT Ethers, uses
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(glycidyl, C12-C16-alkyl, reaction products with nonpolymeric polyamines; production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT Wetting agents
(nonionic; production of alkyl glycidyl ether-capped polyamines suitable for use as)

IT Amines, uses
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(polyamines, nonpolymeric, reaction products with alkyl glycidyl ethers; production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT Antifoaming agents
Surfactants
(production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 56-18-8DP, reaction products with alkyl glycidyl ethers 112-24-3DP, reaction products with alkyl glycidyl ethers 63888-68-6P 488783-16-0P 488783-17-1P 488783-18-2P 488783-19-3P 488783-20-6P 488783-21-7P 488803-37-8P 490035-26-2P 490035-27-3P 490035-28-4P 490035-29-5P 490035-30-8P 491577-26-5P 491577-27-6P 491577-28-7P 491577-29-8P 491577-30-1P 491577-31-2P 491577-32-3P 491577-33-4P
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(production of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 56-18-8, Di(3-aminopropyl)amine 111-40-0, Diethylenetriamine 112-24-3, Ancamine TETA 2426-08-6, Epodil 741 2461-15-6, Epodil 746 160338-56-

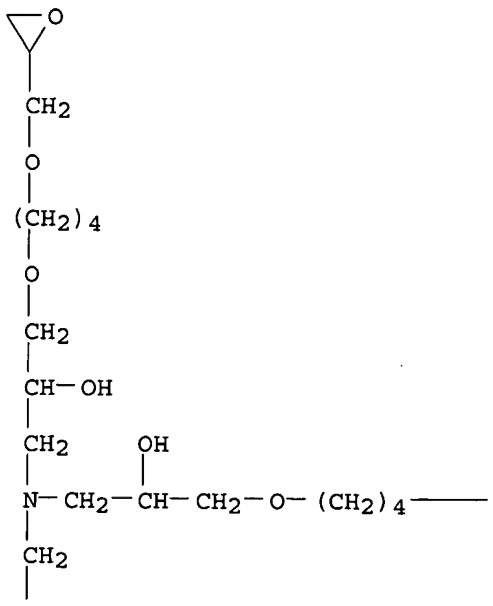
7, Epodil 748
RL: RCT (Reactant); RACT (Reactant or reagent)
(production of alkyl glycidyl ether-capped polyamine antifoaming agents)
IT 577-11-7, Dioctyl sodium sulfosuccinate
RL: TEM (Technical or engineered material use); USES (Uses)
(suppression of foam of; production of alkyl glycidyl ether-capped polyamine antifoaming agents)

L20 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 264627-16-9 REGISTRY
ED Entered STN: 12 May 2000
CN 2,7,26,31-Tetraoxa-11,14,17,20,23-pentaazadotriacontane-9,25-diol, 11,14,17,20,23-pentakis[2-hydroxy-3-[4-(oxiranylmethoxy)butoxy]propyl]-1,32-bis(oxiranyl)- (9CI) (CA INDEX NAME)
MF C78 H149 N5 O28
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RLD.P Roles for non-specific derivatives from patents: PREP (Preparation)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C20	OC2	3	C20	1.30.1	7

PAGE 1-A



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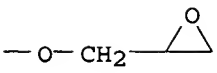

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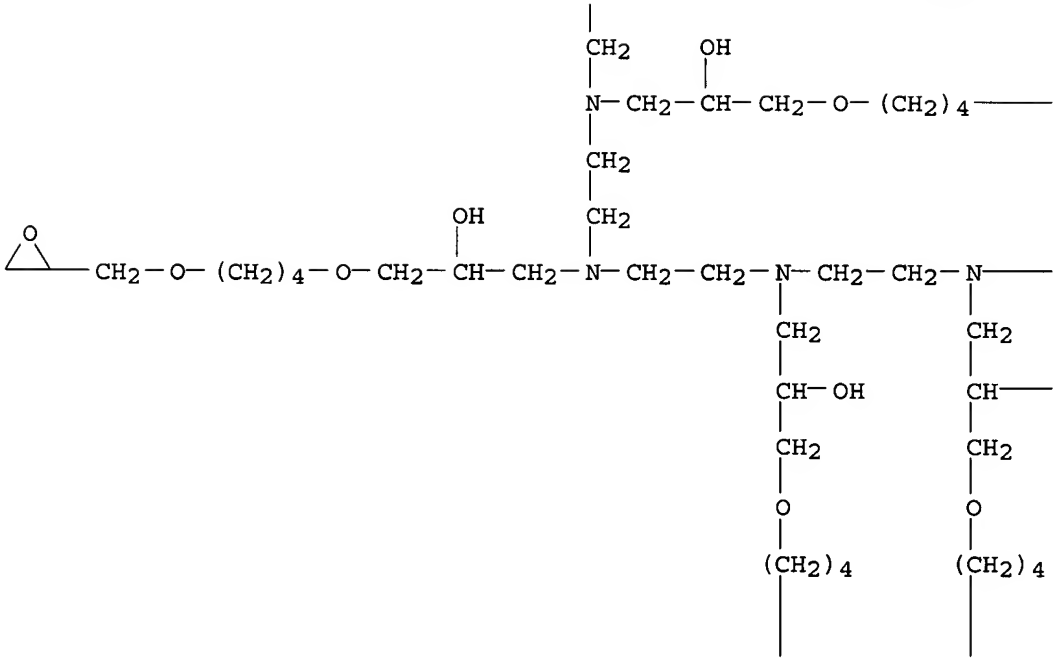
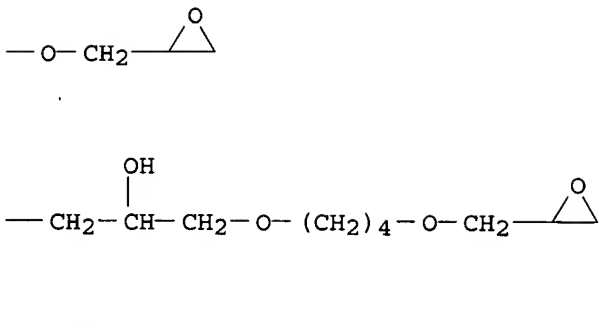
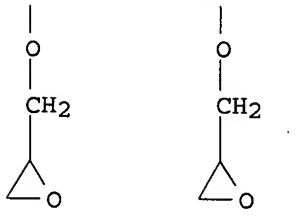






Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	22.44	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	140.47	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	168.24	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	171.06	pH 10 25 deg C	(1)
Boiling Point (BP)	1273.1+/-65.0 deg C	760 Torr	(1)
Density (DEN)	1.199+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	214.58+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	723.7+/-34.3 deg C		(1)
Freely Rotatable Bonds (FRB)	96		(1)
H acceptors (HAC)	33		(1)
H donors (HD)	7		(1)
Hydrogen Donors/Acceptors Sum	40		(1)

(HDAS)			
Koc (KOC)	1.0	pH 1 25 deg C	(1)
Koc (KOC)	1.0	pH 2 25 deg C	(1)
Koc (KOC)	1.0	pH 3 25 deg C	(1)
Koc (KOC)	1.0	pH 4 25 deg C	(1)
Koc (KOC)	1.0	pH 5 25 deg C	(1)
Koc (KOC)	1.0	pH 6 25 deg C	(1)
Koc (KOC)	180.93	pH 7 25 deg C	(1)
Koc (KOC)	1132.38	pH 8 25 deg C	(1)
Koc (KOC)	1356.25	pH 9 25 deg C	(1)
Koc (KOC)	1379.04	pH 10 25 deg C	(1)
logD (LOGD)	-3.49	pH 1 25 deg C	(1)
logD (LOGD)	-2.39	pH 2 25 deg C	(1)
logD (LOGD)	-1.91	pH 3 25 deg C	(1)
logD (LOGD)	-1.85	pH 4 25 deg C	(1)
logD (LOGD)	-1.74	pH 5 25 deg C	(1)
logD (LOGD)	0.02	pH 6 25 deg C	(1)
logD (LOGD)	2.36	pH 7 25 deg C	(1)
logD (LOGD)	3.16	pH 8 25 deg C	(1)
logD (LOGD)	3.23	pH 9 25 deg C	(1)
logD (LOGD)	3.24	pH 10 25 deg C	(1)
logP (LOGP)	3.243+/-0.998	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	1000 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	Unbuffered Water pH 10.39 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.62 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.62 mol/L	Unbuffered Water pH 10.39 25 deg C	(1)
Molar Volume (MVOL)	1337.6+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	1605.03		(1)
pKa (PKA)	13.23+/-0.20	Most Acidic 25 deg C	(1)
pKa (PKA)	7.57+/-0.50	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	351.64 A**2		(1)

Vapor Pressure (VP) |0 Torr |25 deg C |(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:295210 CA
TI Highly branched oligoamides, their preparation and use as epoxy hardeners
IN Moshinsky, Leonid
PA Epox Ltd., Israel
SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C08G083-00
ICS C08G059-54; C08G069-48
CC 42-10 (Coatings, Inks, and Related Products)
Section cross-reference(s): 37
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000022030	A1	20000420	WO 1999-IL540	19991013
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6288208	B1	20010911	US 1999-295320	19990420
	CA 2347200	AA	20000420	CA 1999-2347200	19991013
	AU 9961196	A1	20000501	AU 1999-61196	19991013
	EP 1121386	A1	20010808	EP 1999-947835	19991013
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002527555	T2	20020827	JP 2000-575930	19991013
PRAI	IL 1998-126565	19981014			
	WO 1999-IL540	19991013			

AB The present invention relates to a highly branched polyamide oligomer R[NR1R2]mNR12 (m = 1-5; R = various monovalent groups or epoxy-amide polymers; R2 = linear or branched alkylene, etc.), to the process for preparing such branched oligomers and to different uses thereof. The polyamide oligomers may be used, for example, as epoxy hardeners in the preparation of thermosetting compns., as thermoplastic hot melt adhesives, as adhesion promoters and many other suitable applications.
ST polyamine polyamide branched hardener epoxy
IT Synthetic rubber, uses
RL: NUU (Other use, unclassified); USES (Uses)
(butadiene-isoprene, epoxyurethane-terminated; highly branched oligoamides, their preparation and use as epoxy hardeners)
IT Polyamides, preparation

Polyamides, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(dendrimers; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Polyamines
Polyamines
Polyamines
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(epoxy-polyamide-; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Polyamides, uses
Polyamides, uses
Polyamides, uses
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(epoxy-polyamine-; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Crosslinking agents
(for epoxy resins; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Epoxy resins, uses
RL: NUU (Other use, unclassified); USES (Uses)
(hardeners for; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Coating materials
(highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Castor oil
RL: IMF (Industrial manufacture); PREP (Preparation)
(methanolysis products, reaction products with salicylic acid, reaction products with diethylentriamine, dendripolyamides; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Sunflower oil
RL: IMF (Industrial manufacture); PREP (Preparation)
(methanolysis products, reaction products with terephthalic acid, reaction products with triethylenetetramine, dendripolyamides; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Epoxy resins, uses
Epoxy resins, uses
Epoxy resins, uses
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(polyamide-polyamine-; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT Dendritic polymers
Dendritic polymers
RL: IMF (Industrial manufacture); PREP (Preparation)
(polyamides; highly branched oligoamides, their preparation and use as epoxy hardeners)

IT 69-72-7DP, Salicylic acid, reaction products with castor oil methanolysis products, reaction products with diethylentriamine, dendripolyamides 100-21-0DP, Terephthalic acid, reaction products with sunflower oil methanolysis products, reaction products with triethylene tetramine, dendripolyamides 111-20-6DP, Sebacic acid, reaction products with bean oil methanolysis products, reaction products with triethylene tetramine, dendripolyamides 111-40-0DP, Diethylenetriamine, reaction products with oil-acid adducts, dendripolyamides 112-24-3DP, Triethylene tetramine, reaction products with oil-acid adducts, dendripolyamides 112-57-2DP, Tetra-ethylenepentamine, reaction products with oil-acid adducts, dendripolyamides 124-04-9DP, Adipic acid, reaction products with bean

oil methanolysis products, reaction products with tetraethylenepentamine, dendripolyamides 124-09-4DP, Hexamethylenediamine, adduct with Epon 834, reaction products with polyamides, dendripolyamides 826-62-0DP, reaction products with polyamide cross linking agent 2994-63-0DP, reaction products with polyamides, dendripolyamides, dendripolyamides 3878-43-1DP, reaction products with polyamide-polyamines, dendripolyamides 12624-35-0DP, dendripolyamides 16096-31-4DP, 1,6-Hexanediol diglycidyl ether, reaction products with polyamide-polyamines, dendripolyamides 25068-38-6DP, Epon 834, adduct with hexamethylenediamine, reaction products with polyamides, dendripolyamides 26590-20-5DP, Methyltetrahydrophthalic anhydride, reaction products with polyamide-polyamines, polydendrimers 38294-64-3DP, dendripolyamides 56727-50-5DP, dendripolyamides 136601-29-1DP, Araldite HY 825, reaction products with epoxy resins, dendripolyamides 145249-58-7DP, dendripolyamides 264627-13-6DP, dendripolyamides 264627-14-7DP, dendripolyamides 264627-15-8DP, dendripolyamides 264627-16-9DP, dendripolyamides 264627-17-0DP, dendripolyamides 264627-18-1DP, dendripolyamides 264627-19-2DP, dendripolyamides 264878-36-6DP, dendripolyamides
RL: IMF (Industrial manufacture); PREP (Preparation)
(highly branched oligoamides, their preparation and use as epoxy hardeners)

IT 25610-21-3DP, Diethylene glycol sebacic acid copolymer, reaction products with Epon 828 25667-63-4DP, Diethylene glycol sebacic acid copolymer, sru, reaction products with Epon 828
RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PREP (Preparation); USES (Uses)
(highly branched oligoamides, their preparation and use as epoxy hardeners)

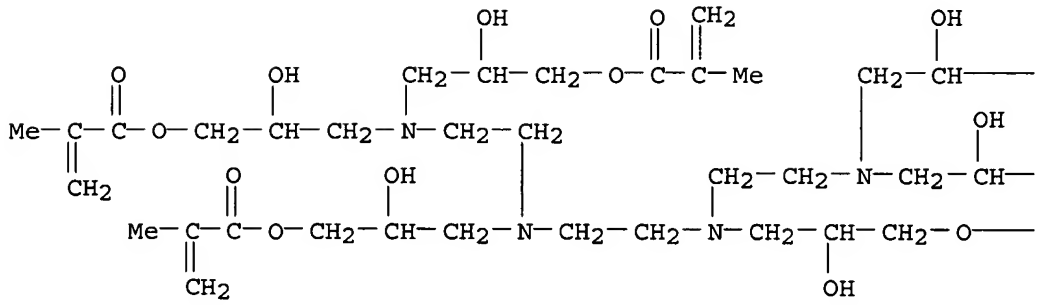
IT 25068-38-6, Epon 828 26142-30-3, Poly (propyleneglycol) diglycidyl ether 68665-19-0, UP-650D 264884-14-2, ELP 812
RL: NUU (Other use, unclassified); USES (Uses)
(highly branched oligoamides, their preparation and use as epoxy hardeners)

IT 101-90-6, Resorcinol diglycidyl ether 107-15-3, 1,2-Ethanediamine, reactions 108-45-2, 1,3-Benzenediamine, reactions 539-48-0, p-Xylylenediamine 826-62-0, 5-Norbornene-2,3-dicarboxylic acid anhydride 1675-54-3 2425-79-8, 1,4-Butanediol diglycidyl ether 2855-13-2, Isophoronediamine 3072-84-2 3114-70-3, 1,4-Cyclohexanediamine 3312-60-5, N-Cyclohexyl-1,3-propanediamine 4403-71-8, 4-Aminobenzylamine 9046-10-0, Poly(propylene glycol)bis(2-aminopropyl)ether 15336-81-9 18799-27-4 22338-32-5 136601-29-1, Araldite HY 825
RL: RCT (Reactant); RACT (Reactant or reagent)
(highly branched oligoamides, their preparation and use as epoxy hardeners)

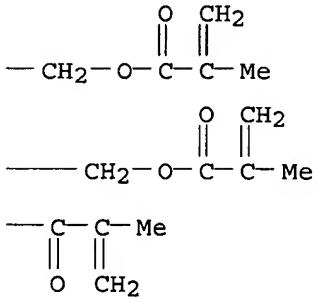
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Allied-Signal; WO 9317062 A 1993 CAPLUS
(2) Renfrew; US 2705223 A 1995 CAPLUS
(3) Sayed-Sweet, Y; JOURNAL OF MATERIALS CHEMISTRY 1997, V7(7) CAPLUS
(4) Waddill; US 4421906 A 1983 CAPLUS

L20 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 253433-70-4 REGISTRY
ED Entered STN: 25 Jan 2000
CN 2-Propenoic acid, 2-methyl-, 1,2-ethanediylbis[[[2-hydroxy-3-[(2-methyl-1-oxo-2-propenyl)oxy]propyl]imino]-2,1-ethanediylnitrilobis(2-hydroxy-3,1-propanediyl)] ester (9CI) (CA INDEX NAME)
MF C48 H78 N4 O18
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: USES (Uses)

PAGE 1-A



PAGE 1-B



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.28	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	3.54	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	8.10	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	25.58	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	90.16	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	4042.20	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	116891.10	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	412375.22	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	501526.66	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	510982.44	pH 10 25 deg C	(1)
Boiling Point (BP)	983.8+/-65.0 deg C	760 Torr	(1)
Density (DEN)	1.207+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	162.54+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	548.8+/-34.3 deg C		(1)
Freely Rotatable Bonds (FRB)	51		(1)
H acceptors (HAC)	22		(1)
H donors (HD)	6		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	28		(1)
Koc (KOC)	1.06	pH 1 25 deg C	(1)

Koc (KOC)	2.94	pH 2 25 deg C	(1)
Koc (KOC)	6.71	pH 3 25 deg C	(1)
Koc (KOC)	21.19	pH 4 25 deg C	(1)
Koc (KOC)	74.71	pH 5 25 deg C	(1)
Koc (KOC)	3349.50	pH 6 25 deg C	(1)
Koc (KOC)	96860.02	pH 7 25 deg C	(1)
Koc (KOC)	341708.41	pH 8 25 deg C	(1)
Koc (KOC)	415582.38	pH 9 25 deg C	(1)
Koc (KOC)	423417.75	pH 10 25 deg C	(1)
logD (LOGD)	2.21	pH 1 25 deg C	(1)
logD (LOGD)	2.66	pH 2 25 deg C	(1)
logD (LOGD)	3.01	pH 3 25 deg C	(1)
logD (LOGD)	3.51	pH 4 25 deg C	(1)
logD (LOGD)	4.06	pH 5 25 deg C	(1)
logD (LOGD)	5.71	pH 6 25 deg C	(1)
logD (LOGD)	7.17	pH 7 25 deg C	(1)
logD (LOGD)	7.72	pH 8 25 deg C	(1)
logD (LOGD)	7.81	pH 9 25 deg C	(1)
logD (LOGD)	7.81	pH 10 25 deg C	(1)
logP (LOGP)	7.818+/-0.849	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.012 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	770 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	240 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	68 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	1.5 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.052 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.015 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.012 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.012 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.013 g/L	Unbuffered Water pH 8.23 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.000012 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	1.00 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.00 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.77 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.24 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.068 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0015 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000052 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000015 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000012 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000012 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000013 mol/L	Unbuffered Water pH 8.23 25 deg C	(1)
Molar Volume (MVOL)	827.4+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	999.15		(1)
pKa (PKA)	12.76+/-0.20	Most Acidic 25 deg C	(1)
pKa (PKA)	7.16+/-0.50	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	292.14 A**2		(1)
Vapor Pressure (VP)	0 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:71495 CA
TI photosensitive paste and manufacture of plasma display panel material
IN Kusano, kazutaka; Ikeda, Norimasa; Horiuchi, Takeshi
PA Toray Industries, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM G03F007-004
ICS G03F007-004; C03C008-14; H01J009-02; H01J011-02
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 35
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2000010268	A2	20000114	JP 1999-102315	19990409
PRAI	JP 1998-110406		19980421		

AB The paste contains inorg. particles and a photosensitive paste containing photosensitive organic compound R1R3NLNR2R4 (R1-2 = substituent having ethylenic unsatd. group; R3-4 = substituent having ethylenic unsatd. group, H, C1-20 alkyl, aryl, aralkyl; L = divalent linkage). The plasma display panel is manufactured by (1) coating the photosensitive paste on a substrate and drying, (2) patterning the composition by photolithog., and (3) firing the patterns for barrier rib formation. Patterns with high aspect ratio and accuracy are obtained.

ST photosensitive paste unsatd amine compd; plasma display panel barrier rib formation

IT Aluminoborosilicate glasses
RL: DEV (Device component use); USES (Uses)
(barium lithium magnesium zinc aluminoborosilicate; photosensitive paste containing unsatd. amine compound and inorg. particles for manufacture of plasma display panel)

IT Plasma display panels
(photosensitive paste containing unsatd. amine compound and inorg. particles for manufacture of plasma display panel)

IT 6197-30-4, 2-Ethylhexyl-2-cyano-3,3-diphenyl acrylate
RL: DEV (Device component use); MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(UV absorbent; photosensitive paste containing unsatd. amine compound and inorg. particles for manufacture of plasma display panel)

IT 35074-77-2
RL: DEV (Device component use); MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(antioxidant; photosensitive paste containing unsatd. amine compound and inorg. particles for manufacture of plasma display panel)

IT 70701-24-5 83372-16-1 253433-68-0 253433-69-1 253433-70-4
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(photosensitive paste containing unsatd. amine compound and inorg. particles for manufacture of plasma display panel)

IT 106-91-2, Glycidyl methacrylate 107-15-3, 1,2-Ethanediamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of unsatd. amine compound)

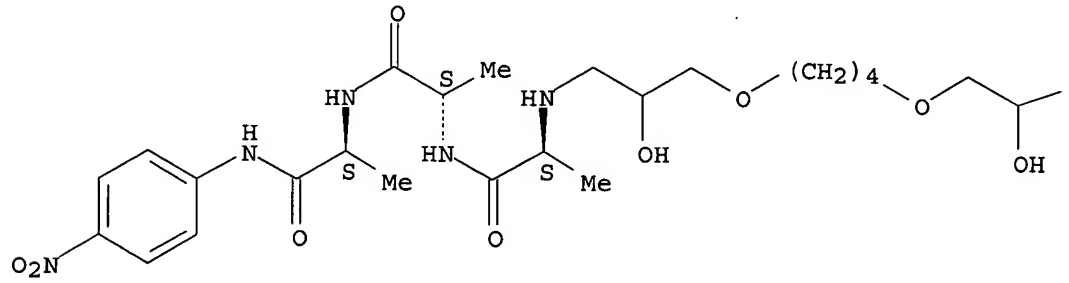
L20 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 173328-48-8 REGISTRY
ED Entered STN: 22 Feb 1996
CN L-Alaninamide, N-[3-[4-(2,3-dihydroxypropoxy)butoxy]-2-hydroxypropyl]-L-alanyl-L-alanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H41 N5 O10
CI COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1

Absolute stereochemistry.

PAGE 1-A



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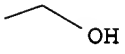


Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE

Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 10 25 deg C	(1)
Boiling Point (BP)	917.8+/-65.0 deg C	760 Torr	(1)
Density (DEN)	1.290+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	139.82+/-3.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	508.9+/-34.3 deg C		(1)
Freely Rotatable Bonds (FRB)	23		(1)
H acceptors (HAC)	15		(1)
H donors (HD)	7		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	22		(1)
Koc (KOC)	1.0	pH 1 25 deg C	(1)
Koc (KOC)	1.0	pH 2 25 deg C	(1)
Koc (KOC)	1.0	pH 3 25 deg C	(1)
Koc (KOC)	1.0	pH 4 25 deg C	(1)
Koc (KOC)	1.0	pH 5 25 deg C	(1)
Koc (KOC)	6.88	pH 6 25 deg C	(1)
Koc (KOC)	20.79	pH 7 25 deg C	(1)
Koc (KOC)	26.08	pH 8 25 deg C	(1)
Koc (KOC)	26.74	pH 9 25 deg C	(1)
Koc (KOC)	26.58	pH 10 25 deg C	(1)
logD (LOGD)	-3.01	pH 1 25 deg C	(1)
logD (LOGD)	-2.99	pH 2 25 deg C	(1)
logD (LOGD)	-2.85	pH 3 25 deg C	(1)
logD (LOGD)	-2.28	pH 4 25 deg C	(1)
logD (LOGD)	-1.37	pH 5 25 deg C	(1)
logD (LOGD)	-0.50	pH 6 25 deg C	(1)
logD (LOGD)	-0.02	pH 7 25 deg C	(1)
logD (LOGD)	0.08	pH 8 25 deg C	(1)
logD (LOGD)	0.09	pH 9 25 deg C	(1)
logD (LOGD)	0.09	pH 10 25 deg C	(1)
logP (LOGP)	0.096+/-0.872	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.20 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	250 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	240 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	180 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	47 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	5.7 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.80 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.26 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.21 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.20 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.20 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.20 g/L	Unbuffered Water pH 8.50 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.00035 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.44 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.42 mol/L	pH 2 25 deg C	(1)

Molar Solubility (SLB.MOL)	0.31 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.083 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.010 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0014 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00045 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00036 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00035 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00035 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00035 mol/L	Unbuffered Water pH 8.50 25 deg C	(1)
Molar Volume (MVOL)	442.7+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	571.62		(1)
pKa (PKA)	12.47+/-0.70	Most Acidic 25 deg C	(1)
pKa (PKA)	6.46+/-0.38	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	195.55 A**2		(1)
Vapor Pressure (VP)	0 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

L20 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 74029-26-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Sepharose CL 4B, (14S,17S,20S)-2,11-dihydroxy-14,17,20-trimethyl-21-[(4-nitrophenyl)amino]-15,18,21-trioxo-4,9-dioxa-13,16,19-triazaheneicos-1-yl ether (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H41 N5 O10 . x Unspecified
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study)

Ring System Data

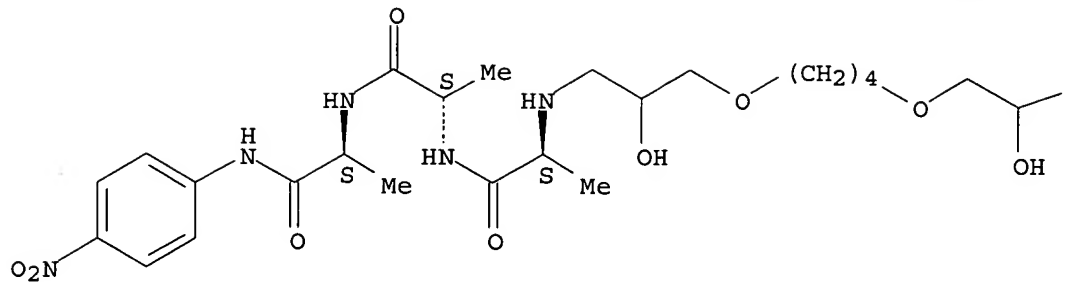
Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1 in CM 1

CM 1

CRN 173328-48-8
CMF C25 H41 N5 O10

Absolute stereochemistry.

PAGE 1-A



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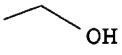


CM 2

CRN 62610-50-8
CMF Unspecified
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 93:21365 CA
TI One-step purification of human leukocyte elastase by biospecific affinity chromatography at subzero temperatures
AU Andersson, Kristoffer K.; Balny, Claude; Douzou, Pierre; Bieth, Joseph G.
CS INSERM, Montpellier, 34033, Fr.
SO Journal of Chromatography (1980), 192(1), 236-9
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
CC 7-2 (Enzymes)
AB Human leukocyte elastase was purified from a crude granule extract by affinity chromatog. on L-trialanine-p-nitroanilide coupled to diglycidyl ether-activated Sepharose 6B CL at subzero temps. (nonturnover conditions). Crude granular extract (100 μL) was mixed with 500 μL of 0.1M NaOAc buffer, pH 5, containing 4M NaCl. The mixture was cooled to -14° and applied to the affinity column at a flow rate of 1 mL/h. After 1 h, in which complete adsorption of enzyme was achieved, impurities were eluted with 20 mL of the same buffer. Elastase was then desorbed with a mixture of equal vols. of ethylene glycol and 0.2M NaOAc buffer (paH 5.0) without NaCl. The elution profile showed a single peak with good coincidence of protein and activity; the activity yield was .apprx.85%.
ST elastase leukocyte purifn affinity chromatog
IT Leukocyte

(elastase of, affinity chromatog. in purification of)
IT 74029-26-8
RL: BIOL (Biological study)
(elastase of leukocyte affinity chromatog. on, at subzero temps.)
IT 9004-06-2P
RL: PREP (Preparation)
(of leukocyte, purification of, affinity chromatog. at low temps. in)

L20 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 69458-28-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Agarose, 2,11-dihydroxy-14,17,20-trimethyl-21-[(4-nitrophenyl)amino]-15,18,21-trioxo-4,9-dioxa-13,16,19-triazaheneicos-1-yl ether (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H41 N5 O10 . x Unspecified
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study)

Ring System Data

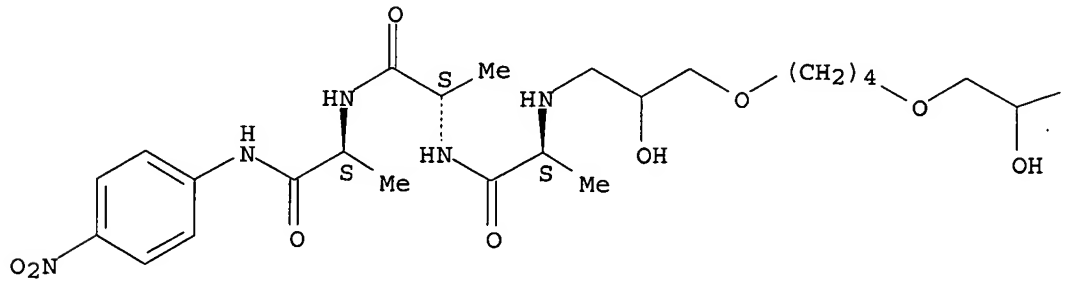
Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1 in CM 1

CM 1

CRN 173328-48-8
CMF C25 H41 N5 O10

Absolute stereochemistry.

PAGE 1-A



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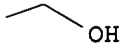

CM 2

CRN 9012-36-6
CMF Unspecified
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 90:99088 CA
TI Affinity chromatography at sub-zero temperatures. A model study with porcine pancreatic elastase
AU Balny, Claude; Le Doucen, Christian; Douzou, Pierre
CS INSERM, Montpellier, Fr.
SO Journal of Chromatography (1979), 168(1), 133-8
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
CC 7-2 (Enzymes)
Section cross-reference(s): 9
AB A new variety of affinity chromatog. of enzymes is described which consists of building up an affinity adsorbent composed of a real substrate. The chromatog. is performed at a sub-zero temperature where the turnover of the enzyme is very low or stopped. As a model system Sepharose-bound L-trialanine p-nitroanilide was used for the affinity binding of porcine pancreatic elastase, which was adsorbed to the column in a hypersaline medium at -14° and eluted from the column at the same temperature using 50% ethylene glycol. The affinity adsorbent proved to be very specific as it did not retain trypsin, chymotrypsin, and ovalbumin and retained only 20% of cytochrome c.
ST chromatog affinity adsorbent substrate enzyme; elastase affinity chromatog
IT Enzymes
RL: PROC (Process)
(affinity chromatog. of, on adsorbent containing substrate at sub-zero temps.)
IT Adsorbents
(for enzymes, substrate-containing, for low temperature chromatog.)
IT Cold, chemical and physical effects
(on affinity chromatog. of enzyme)
IT Chromatography, column and liquid
(affinity, at sub-zero temps., of enzymes with affinity adsorbent substrate)
IT 9004-06-2
RL: PROC (Process)
(affinity chromatog. of, on substrate-containing adsorbent at sub-zero temps.)
IT 69458-28-2
RL: BIOL (Biological study)
(elastase affinity chromatog. on, at sub-zero temps.)
IT 60354-61-2D, reaction products with Sepharose
RL: BIOL (Biological study)
(in affinity chromatog. of elastase at sub-zero temps.)

L20 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 63888-76-6 REGISTRY

ED Entered STN: 16 Nov 1984
CN 9,26-Dioxa-13,16,19,22-tetraazatetratriacontane-11,24-diol, hydrochloride (9CI) (CA INDEX NAME)
MF C28 H62 N4 O4 . x Cl H
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)
CRN (63888-71-1)

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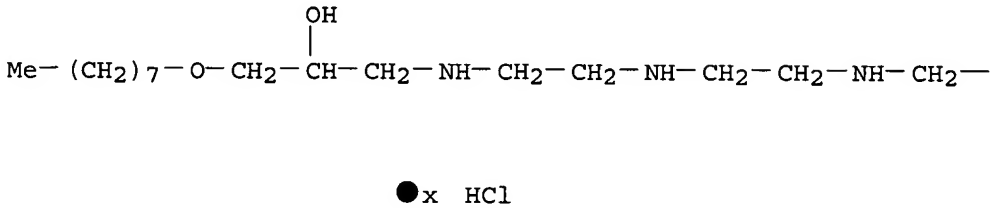

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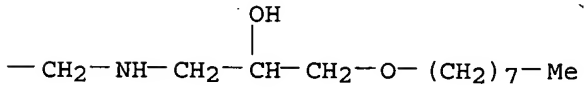


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 87:151695 CA
TI Bactericidal alkylenepolyamines
IN Ito, Hirohiko; Mizuno, Yasushi; Yamamoto, Tsuneo
PA Takemoto Oil and Fat Co., Ltd., Japan
SO Jpn. Tokkyo Koho, 5 pp.
CODEN: JAXXAD
DT Patent
LA Japanese
IC C07C093-04
CC 23-7 (Aliphatic Compounds)
Section cross-reference(s): 63
FAN.CNT 1

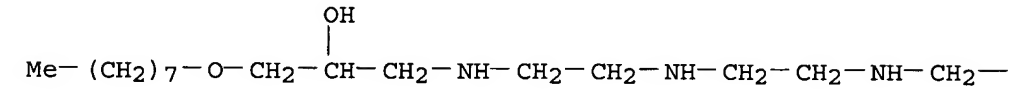
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 52018047	B4	19770519	JP 1972-114766	19721117
	JP 49074412	A2	19740718		
PRAI	JP 1972-114766		19721117		

AB R1R2NZ(NR3Z)nNR4R5 (I; R1-5 = H, 3-alkoxy-2-hydroxypropyl; Z = C2-3 alkylene, n = 1, 2), effective bactericides and fungicides against Salmonella typhosa, etc., were prepared by reaction of H2NZ(NHZ)nNH2 (II) with alkyl glycidyl ethers. Thus, 29 parts II (Z = CH2CH2, n = 1) was heated with 70 parts 2-ethylhexyl glycidyl ether at 180° to give the corresponding I, the HCl salt of which was 90 times more effective against Salmonella typhosa than was PhOH.
ST alkoxyhydroxyalkylenepolyamine bactericide fungicide; alkylenepolyamine bactericide fungicide

IT Bactericides, Disinfectants and Antiseptics
Fungicides and Fungistats
(alkoxyhydroxyalkylenepolyamines)
IT 63870-93-9P 63870-95-1P 63870-96-2P 63888-68-6P 63888-69-7P
63888-70-0P 63888-71-1P 63888-72-2P 63888-73-3P 63888-74-4P
63888-75-5P 63888-76-6P 63888-77-7P 63888-78-8P 63928-92-7P
63928-93-8P 64117-57-3P 64117-58-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 111-40-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (ethylhexyloxy)oxirane)
IT 2461-15-6 29756-57-8 63870-94-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethylenetriamine)
IT 105-83-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethylhexyl glycidyl ether)
IT 112-24-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with octyl glycidyl ether)

L20 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 63888-71-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 9,26-Dioxa-13,16,19,22-tetraazatetratriacontane-11,24-diol (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H62 N4 O4
CI COM
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)

PAGE 1-A



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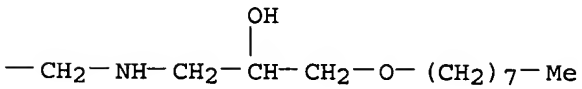


Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE

Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	3.38	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	131.89	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1084.93	pH 10 25 deg C	(1)
Boiling Point (BP)	627.2+/-55.0 deg C	760 Torr	(1)
Density (DEN)	0.970+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	106.39+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	333.1+/-31.5 deg C		(1)
Freely Rotatable Bonds (FRB)	33		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	6		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	14		(1)
Koc (KOC)	1.0	pH 1 25 deg C	(1)
Koc (KOC)	1.0	pH 2 25 deg C	(1)
Koc (KOC)	1.0	pH 3 25 deg C	(1)
Koc (KOC)	1.0	pH 4 25 deg C	(1)
Koc (KOC)	1.0	pH 5 25 deg C	(1)
Koc (KOC)	1.0	pH 6 25 deg C	(1)
Koc (KOC)	1.0	pH 7 25 deg C	(1)
Koc (KOC)	13.25	pH 8 25 deg C	(1)
Koc (KOC)	517.26	pH 9 25 deg C	(1)
Koc (KOC)	4254.81	pH 10 25 deg C	(1)
logD (LOGD)	-1.38	pH 1 25 deg C	(1)
logD (LOGD)	-1.21	pH 2 25 deg C	(1)
logD (LOGD)	-0.74	pH 3 25 deg C	(1)
logD (LOGD)	-0.42	pH 4 25 deg C	(1)
logD (LOGD)	-0.14	pH 5 25 deg C	(1)
logD (LOGD)	0.35	pH 6 25 deg C	(1)
logD (LOGD)	0.68	pH 7 25 deg C	(1)
logD (LOGD)	1.88	pH 8 25 deg C	(1)
logD (LOGD)	3.48	pH 9 25 deg C	(1)
logD (LOGD)	4.39	pH 10 25 deg C	(1)
logP (LOGP)	4.692+/-0.781	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.029 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	633 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	300 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	18 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.47 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.057 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.067 g/L	Unbuffered Water pH 9.88 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.000056 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	1.93 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.93 mol/L	pH 2 25 deg C	(1)

Molar Solubility (SLB.MOL)	1.93 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.93 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.93 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.22 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.57 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.035 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00091 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00011 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00013 mol/L	Unbuffered Water pH 9.88 25 deg C	(1)
Molar Volume (MVOL)	534.4+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	518.82		(1)
pKa (PKA)	13.73+/-0.20	Most Acidic 25 deg C	(1)
pKa (PKA)	9.88+/-0.19	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	107.04 A**2		(1)
Vapor Pressure (VP)	2.33E-18 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 87:151695 CA
TI Bactericidal alkylenepolyamines
IN Ito, Hirohiko; Mizuno, Yasushi; Yamamoto, Tsuneo
PA Takemoto Oil and Fat Co., Ltd., Japan
SO Jpn. Tokkyo Koho, 5 pp.
CODEN: JAXXAD
DT Patent
LA Japanese
IC C07C093-04
CC 23-7 (Aliphatic Compounds)
Section cross-reference(s): 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 52018047	B4	19770519	JP 1972-114766	19721117
	JP 49074412	A2	19740718		
PRAI	JP 1972-114766		19721117		

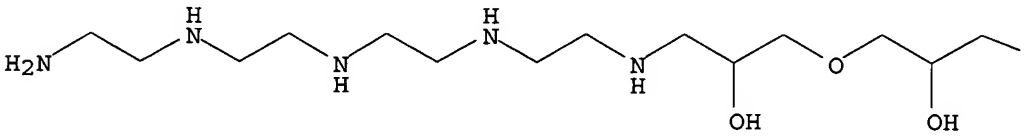
AB R1R2NZ(NR3Z)nNR4R5 (I; R1-5 = H, 3-alkoxy-2-hydroxypropyl; Z = C2-3 alkylene, n = 1, 2), effective bactericides and fungicides against Salmonella typhosa, etc., were prepared by reaction of H2NZ(NHZ)nNH2 (II) with alkyl glycidyl ethers. Thus, 29 parts II (Z = CH2CH2, n = 1) was heated with 70 parts 2-ethylhexyl glycidyl ether at 180° to give the corresponding I, the HCl salt of which was 90 times more effective against Salmonella typhosa than was PhOH.
ST alkoxyhydroxyalkylenepolyamine bactericide fungicide; alkylenepolyamine bactericide fungicide
IT Bactericides, Disinfectants and Antiseptics
Fungicides and Fungistats
(alkoxyhydroxyalkylenepolyamines)

IT 63870-93-9P 63870-95-1P 63870-96-2P 63888-68-6P 63888-69-7P
63888-70-0P 63888-71-1P 63888-72-2P 63888-73-3P 63888-74-4P
63888-75-5P 63888-76-6P 63888-77-7P 63888-78-8P 63928-92-7P
63928-93-8P 64117-57-3P 64117-58-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 111-40-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (ethylhexyloxy)oxirane)
IT 2461-15-6 29756-57-8 63870-94-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethylenetriamine)
IT 105-83-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethylhexyl glycidyl ether)
IT 112-24-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with octyl glycidyl ether)

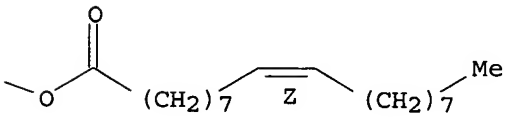
L20 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 37997-92-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN 9-Octadecenoic acid (9Z)-, 19-amino-2,6-dihydroxy-4-oxa-8,11,14,17-tetraazanonadec-1-yl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9-Octadecenoic acid (Z)-, 19-amino-2,6-dihydroxy-4-oxa-8,11,14,17-tetraazanonadec-1-yl ester
FS STEREOSEARCH
MF C32 H67 N5 O5
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
DT.CA CAplus document type: Patent
RL.P Roles from patents: USES (Uses)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



10/618117

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	37.29	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	904.10	pH 10 25 deg C	(1)
Boiling Point (BP)	707.8+/-60.0 deg C	760 Torr	(1)
Density (DEN)	1.011+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	118.31+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	381.8+/-32.9 deg C		(1)
Freely Rotatable Bonds (FRB)	38		(1)
H acceptors (HAC)	10		(1)
H donors (HD)	8		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	18		(1)
Koc (KOC)	1.0	pH 1 25 deg C	(1)
Koc (KOC)	1.0	pH 2 25 deg C	(1)
Koc (KOC)	1.0	pH 3 25 deg C	(1)
Koc (KOC)	1.0	pH 4 25 deg C	(1)
Koc (KOC)	1.0	pH 5 25 deg C	(1)
Koc (KOC)	1.0	pH 6 25 deg C	(1)
Koc (KOC)	1.0	pH 7 25 deg C	(1)
Koc (KOC)	1.34	pH 8 25 deg C	(1)
Koc (KOC)	130.88	pH 9 25 deg C	(1)
Koc (KOC)	3173.14	pH 10 25 deg C	(1)
logD (LOGD)	-2.15	pH 1 25 deg C	(1)
logD (LOGD)	-1.91	pH 2 25 deg C	(1)
logD (LOGD)	-1.23	pH 3 25 deg C	(1)
logD (LOGD)	-0.51	pH 4 25 deg C	(1)
logD (LOGD)	-0.23	pH 5 25 deg C	(1)
logD (LOGD)	-0.16	pH 6 25 deg C	(1)
logD (LOGD)	0.03	pH 7 25 deg C	(1)
logD (LOGD)	0.99	pH 8 25 deg C	(1)
logD (LOGD)	2.98	pH 9 25 deg C	(1)
logD (LOGD)	4.37	pH 10 25 deg C	(1)
logP (LOGP)	4.915+/-0.881	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.024 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	999 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	180 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	1.7 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.072 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.078 g/L	Unbuffered Water pH 9.97 25 deg C	(1)
Molar Intrinsic Solubility	0.000040 mol/L	25 deg C	(1)

(ISLB.MOL)			
Molar Solubility (SLB.MOL)	1.66 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.66 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.66 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.66 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.66 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.66 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.66 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.30 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0029 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00012 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00013 mol/L	Unbuffered Water pH 9.97 25 deg C	(1)
Molar Volume (MVOL)	594.9+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	601.90		(1)
pKa (PKA)	13.09+/-0.20	Most Acidic 25 deg C	(1)
pKa (PKA)	9.77+/-0.19	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	150.13 A**2		(1)
Vapor Pressure (VP)	3.77E-23 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 77:78458 CA
TI Corrosion-inhibited aqueous alkaline solutions for cleaning a ferrous metal surface
IN Teumac, Fred Norman; Harriman, Lester W.
PA Dow Chemical Co.
SO U.S., 4 pp.
CODEN: USXXAM
DT Patent
LA English
IC C23G; B08B
NCL 134002000
CC 55-9 (Ferrous Metals and Alloys)
Section cross-reference(s): 46
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3668009	A	19720606	US 1970-28079	19700413
PRAI	US 1970-28079	19700413			

AB Hard deposits, e.g. boiler scale, are removed from ferrous surfaces by contact with aqueous alkaline cleaning solns. containing 0.1-40 weight % of an ammoniated polycarboxylic acid complexing agent. A corrosion inhibitor in an amount of 0.0005-0.1 weight % is added to the cleaning solution The corrosion inhibitor has the formula RCO[OCH2CH(OH)CH2]aNH(CH2CH2NH)bH, in which R is a C12-18 alkyl or alkenyl group, a is 1 or 2, and b is 1-5. Ammoniated EDTA is claimed as a complexing agent and thioethylamine, Na

mercaptobenzothiazole, bis(ethylamine) disulfide, and thiazolidine are claimed as synergistic additives to the inhibited cleaning solution These S compds. are added in amts. of 0.01-0.1 weight %.

ST corrosion inhibited ferrous cleaners; thioethylamine corrosion inhibitor; thiazolidine corrosion inhibitor; mercaptobenzothizole sodium corrosion inhibitor; bisethylamine disulfide corrosion inhibitor; amine corrosion inhibitor steel; steel cleaner corrosion inhibited

IT Carboxylic acids, compounds
RL: USES (Uses)
(ammonium salts, corrosion inhibitors, for steam boiler cleaning)

IT Scale (coating)
(boiler, removal of, corrosion inhibitor-containing alkaline solns. for)

IT Corrosion inhibitors
(for steel, in cleaning of steam boilers)

IT Amines, uses and miscellaneous
RL: USES (Uses)
(poly-, corrosion inhibitor, for steam boiler cleaning)

IT Boilers
(steam, cleaning solns. containing corrosion inhibitors for)

IT Fatty acids, uses and miscellaneous
RL: USES (Uses)
(tall oil, corrosion inhibitor, for steam boiler cleaning)

IT 12597-69-2, uses and miscellaneous
RL: USES (Uses)
(cleaning of mild, in steam boilers, inhibitors for)

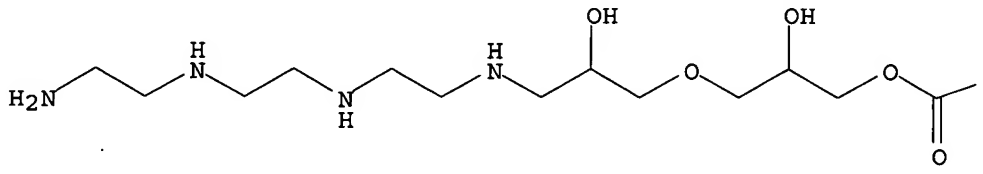
IT 51-85-4 60-23-1 149-30-4 504-78-9 7379-26-2 37340-75-3 37340-76-4 37997-83-4 37997-84-5 37997-85-6 37997-86-7 37997-87-8 37997-88-9 37997-89-0 37997-90-3 37997-91-4 37997-92-5
RL: USES (Uses)
(corrosion inhibitor, for steam boiler cleaning)

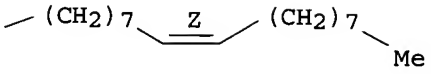
IT 106-89-8, uses and miscellaneous
RL: USES (Uses)
(corrosion inhibitors containing, for steam boiler cleaning)

L20 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 37997-91-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN 9-Octadecenoic acid (9Z)-, 16-amino-2,6-dihydroxy-4-oxa-8,11,14-triazahexadec-1-yl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9-Octadecenoic acid (Z)-, 16-amino-2,6-dihydroxy-4-oxa-8,11,14-triazahexadec-1-yl ester
FS STEREOSEARCH
MF C30 H62 N4 O5
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
DT.CA CAplus document type: Patent
RL.P Roles from patents: USES (Uses)

Double bond geometry as shown.

PAGE 1-A





Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	3.42	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	158.95	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	2012.97	pH 10 25 deg C	(1)
Boiling Point (BP)	672.7+/-55.0 deg C	760 Torr	(1)
Density (DEN)	1.010+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	113.07+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	360.6+/-31.5 deg C		(1)
Freely Rotatable Bonds (FRB)	35		(1)
H acceptors (HAC)	9		(1)
H donors (HD)	7		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	16		(1)
Koc (KOC)	1.0	pH 1 25 deg C	(1)
Koc (KOC)	1.0	pH 2 25 deg C	(1)
Koc (KOC)	1.0	pH 3 25 deg C	(1)
Koc (KOC)	1.0	pH 4 25 deg C	(1)
Koc (KOC)	1.0	pH 5 25 deg C	(1)
Koc (KOC)	1.0	pH 6 25 deg C	(1)
Koc (KOC)	1.36	pH 7 25 deg C	(1)
Koc (KOC)	10.31	pH 8 25 deg C	(1)
Koc (KOC)	479.15	pH 9 25 deg C	(1)
Koc (KOC)	6068.11	pH 10 25 deg C	(1)
logD (LOGD)	-0.85	pH 1 25 deg C	(1)
logD (LOGD)	-0.65	pH 2 25 deg C	(1)
logD (LOGD)	-0.17	pH 3 25 deg C	(1)
logD (LOGD)	0.11	pH 4 25 deg C	(1)
logD (LOGD)	0.36	pH 5 25 deg C	(1)
logD (LOGD)	0.85	pH 6 25 deg C	(1)
logD (LOGD)	1.14	pH 7 25 deg C	(1)
logD (LOGD)	2.02	pH 8 25 deg C	(1)
logD (LOGD)	3.68	pH 9 25 deg C	(1)
logD (LOGD)	4.79	pH 10 25 deg C	(1)
logP (LOGP)	5.221+/-0.772	25 deg C	(1)

Mass Intrinsic Solubility (ISLB.MASS)	0.011 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	1000 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	821 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	270 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	130 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	16 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.35 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.027 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.045 g/L	Unbuffered Water pH 9.73 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.000020 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	1.79 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.79 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.79 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.79 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	1.47 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.48 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.24 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.029 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00062 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000049 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000081 mol/L	Unbuffered Water pH 9.73 25 deg C	(1)
Molar Volume (MVOL)	553.0+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	558.84		(1)
pKa (PKA)	13.09+/-0.20	Most Acidic 25 deg C	(1)
pKa (PKA)	9.77+/-0.19	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	138.10 A**2		(1)
Vapor Pressure (VP)	5.61E-21 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 77:78458 CA
TI Corrosion-inhibited aqueous alkaline solutions for cleaning a ferrous metal surface
IN Teumac, Fred Norman; Harriman, Lester W.
PA Dow Chemical Co.
SO U.S., 4 pp.
CODEN: USXXAM
DT Patent
LA English
IC C23G; B08B

NCL 134002000
CC 55-9 (Ferrous Metals and Alloys)
Section cross-reference(s): 46
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3668009	A	19720606	US 1970-28079	19700413
PRAI	US 1970-28079	19700413			

AB Hard deposits, e.g. boiler scale, are removed from ferrous surfaces by contact with aqueous alkaline cleaning solns. containing 0.1-40 weight % of an ammoniated polycarboxylic acid complexing agent. A corrosion inhibitor in an amount of 0.0005-0.1 weight % is added to the cleaning solution The corrosion inhibitor has the formula RCO[OCH2CH(OH)CH2]aNH(CH2CH2NH)bH, in which R is a C12-18 alkyl or alkenyl group, a is 1 or 2, and b is 1-5. Ammoniated EDTA is claimed as a complexing agent and thioethylamine, Na mercaptobenzothiazole, bis(ethylamine) disulfide, and thiazolidine are claimed as synergistic additives to the inhibited cleaning solution These S compds. are added in amts. of 0.01-0.1 weight %.
ST corrosion inhibited ferrous cleaners; thioethylamine corrosion inhibitor; thiazolidine corrosion inhibitor; mercaptobenzothizole sodium corrosion inhibitor; bisethylamine disulfide corrosion inhibitor; amine corrosion inhibitor steel; steel cleaner corrosion inhibited
IT Carboxylic acids, compounds
RL: USES (Uses)
(ammonium salts, corrosion inhibitors, for steam boiler cleaning)
IT Scale (coating)
(boiler, removal of, corrosion inhibitor-containing alkaline solns. for)
IT Corrosion inhibitors
(for steel, in cleaning of steam boilers)
IT Amines, uses and miscellaneous
RL: USES (Uses)
(poly-, corrosion inhibitor, for steam boiler cleaning)
IT Boilers
(steam, cleaning solns. containing corrosion inhibitors for)
IT Fatty acids, uses and miscellaneous
RL: USES (Uses)
(tall oil, corrosion inhibitor, for steam boiler cleaning)
IT 12597-69-2, uses and miscellaneous
RL: USES (Uses)
(cleaning of mild, in steam boilers, inhibitors for)
IT 51-85-4 60-23-1 149-30-4 504-78-9 7379-26-2 37340-75-3 37340-76-4 37997-83-4 37997-84-5 37997-85-6 37997-86-7 37997-87-8 37997-88-9 37997-89-0 37997-90-3 37997-91-4 37997-92-5
RL: USES (Uses)
(corrosion inhibitor, for steam boiler cleaning)
IT 106-89-8, uses and miscellaneous
RL: USES (Uses)
(corrosion inhibitors containing, for steam boiler cleaning)

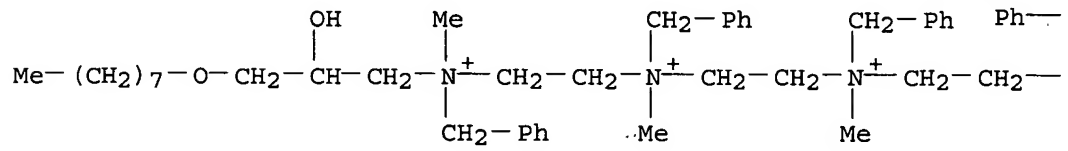
L20 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2006 ACS on STN
RN 36611-09-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,2-Ethanediaminium, N,N'-bis[2-[[2-hydroxy-3-(octyloxy)propyl]methyl(phenylmethyl)ammonio]ethyl]-N,N'-dimethyl-N,N'-bis(phenylmethyl)- (9CI) (CA INDEX NAME)
MF C60 H98 N4 O4
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL
DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	4

PAGE 1-A



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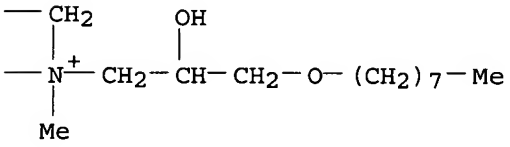

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 77:74820 CA
TI Antibacterial (2-hydroxyalkyl)benzylmethylammonium bromides
IN Temple, Robert D.
PA Procter and Gamble Co.
SO Ger. Offen., 30 pp.
CODEN: GWXXBX
DT Patent
LA German
IC C07C; A61L
CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 46
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2151719	A	19720420	DE 1971-2151719	19711018
	US 3719711	A	19730306	US 1970-82067	19701019
	FR 2111700	A5	19720609	FR 1971-37370	19711018
	FR 2111700	B1	19750606		
	GB 1322636	A	19730711	GB 1971-48369	19711018
PRAI	US 1970-82067	19701019			

GI For diagram(s), see printed CA Issue.
AB Six title compds. RCH2CH(OH)-[CH2N+Me(CH2Ph)CH2]nCH(OH)CH2R Brn- (I; n = 2-4s R = C8H17O or C9H19), useful as antibact-dimethyl-ethylenediamine (II), N,N',N''-trimethyldiethylenetriamine, or N,N',N'',N'''-

tetramethyltriethylenetetramine with III and PhCH2Br (IV). Thus, refluxing II and III (R = C8H17O) in EtOH 16 hr, addition of IV, and refluxing 24 hr gave I (R = C8H17O, n = 2).

ST hydroxyalkylammonium bromide bactericide; ammonium benzylhydroxyalkyl; soap bactericide hydroxyalkylammonium; detergent bactericide hydroxyalkylammonium

IT Detergents
(bactericides for, benzyl(hydroxyalkyl)methylammonium bromides as)

IT Soaps
RL: RCT (Reactant); RACT (Reactant or reagent)
(bactericides for, benzyl(hydroxyalkyl)methylammonium bromides as)

IT Bactericides, Disinfectants and Antiseptics
(benzyl(hydroxyalkyl)methylammonium bromides, for detergents)

IT 36557-85-4P 36557-86-5P 36557-87-6P 36557-88-7P 36611-08-2P 36611-09-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 105-78-2 105-84-0 110-70-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzyl bromide and ethoxides)

IT 2855-19-8 3385-66-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethylene polyamines and benzyl bromide)

IT 100-39-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethylene polyamines and epoxides)

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